FIGURES

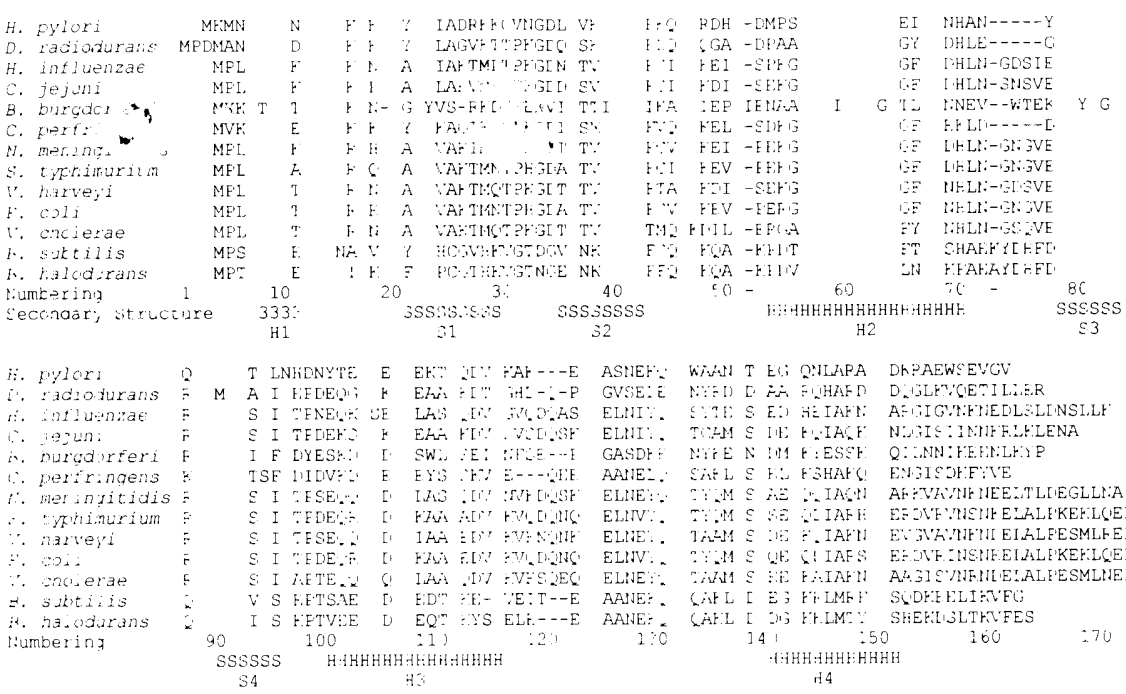


Figure 1 Sequence alignment of LuxS proteins. Color coding: red = greater than 92% identity (or homology in the case of F/Y, S/T, or D/E) and green = hydrophobic residues (A/V/I/L/M/W/Y/F). At the bottom is indicated the residue numbering employed as well as the common secondary structure elements determined in this invention with 3 = 3/10 helix, S = beta strand, and H = alpha helix.

FIG. 2. Represenatative diffraction image from a *H. pylori* LuxS crystal analyzed in this patent.

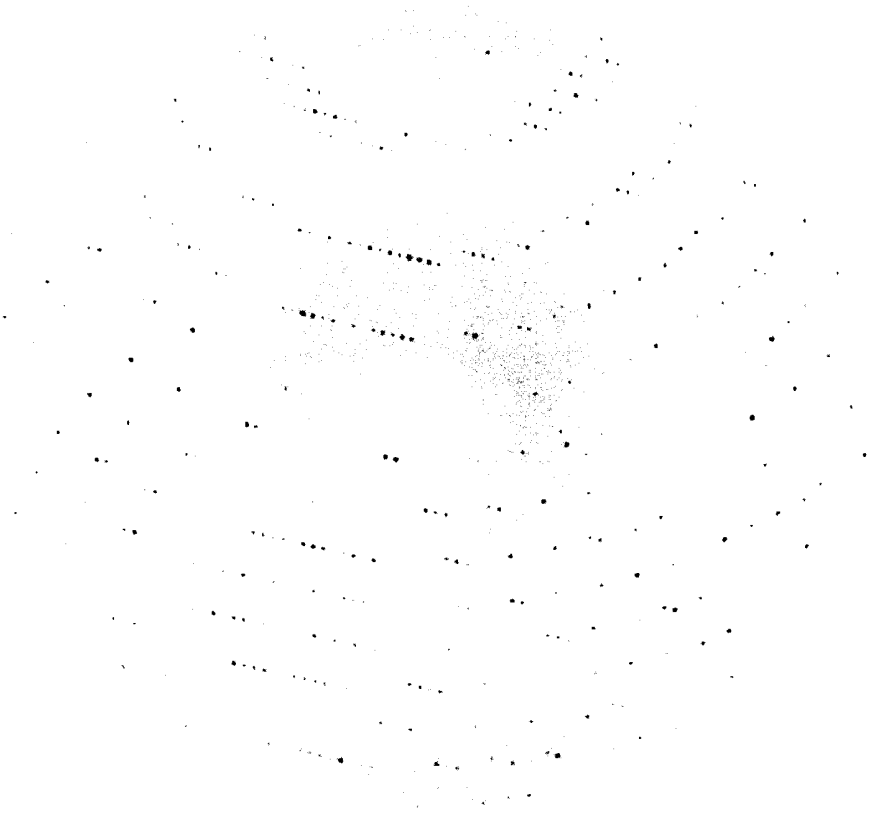


FIG 3. Represenatative diffraction image from a *H.influenzaei* LuxS crystal analyzed in this patent.

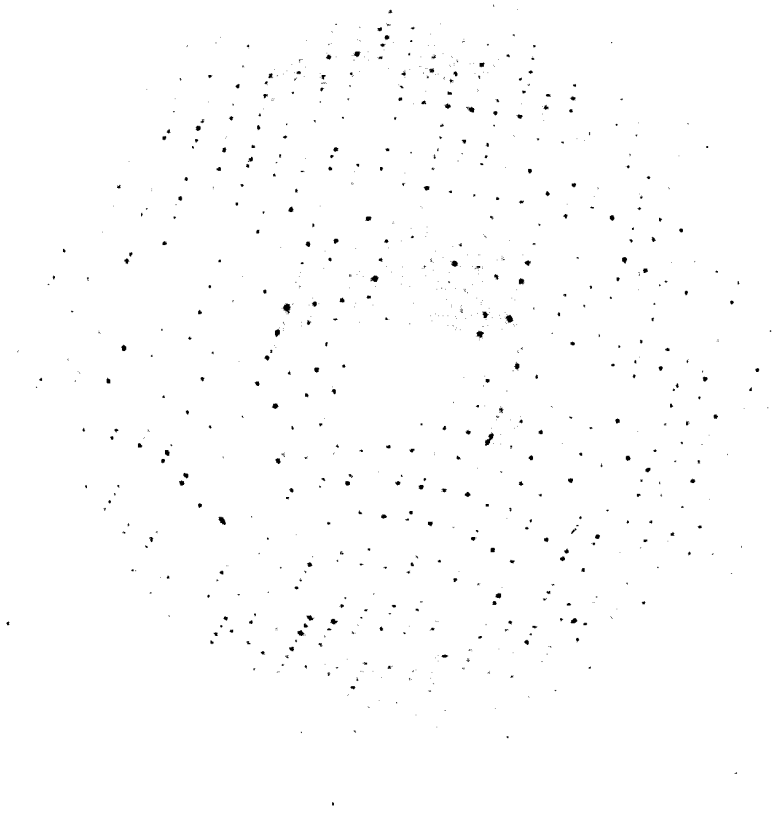


FIG 4. Represenatative diffraction image from $P2_1$ spacegroup *D. radiodurans* LuxS crystals analyzed in this patent.

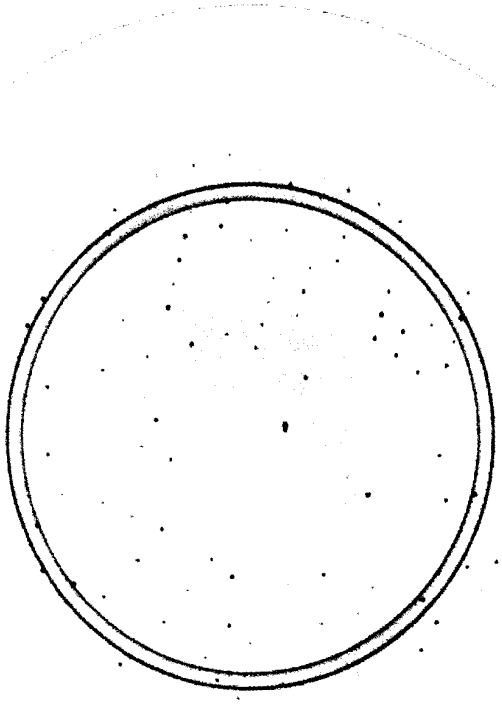


FIG 5. Represenatative diffraction image from C2 spacegroup *D. radiodurans* LuxS crystals analyzed in this patent.

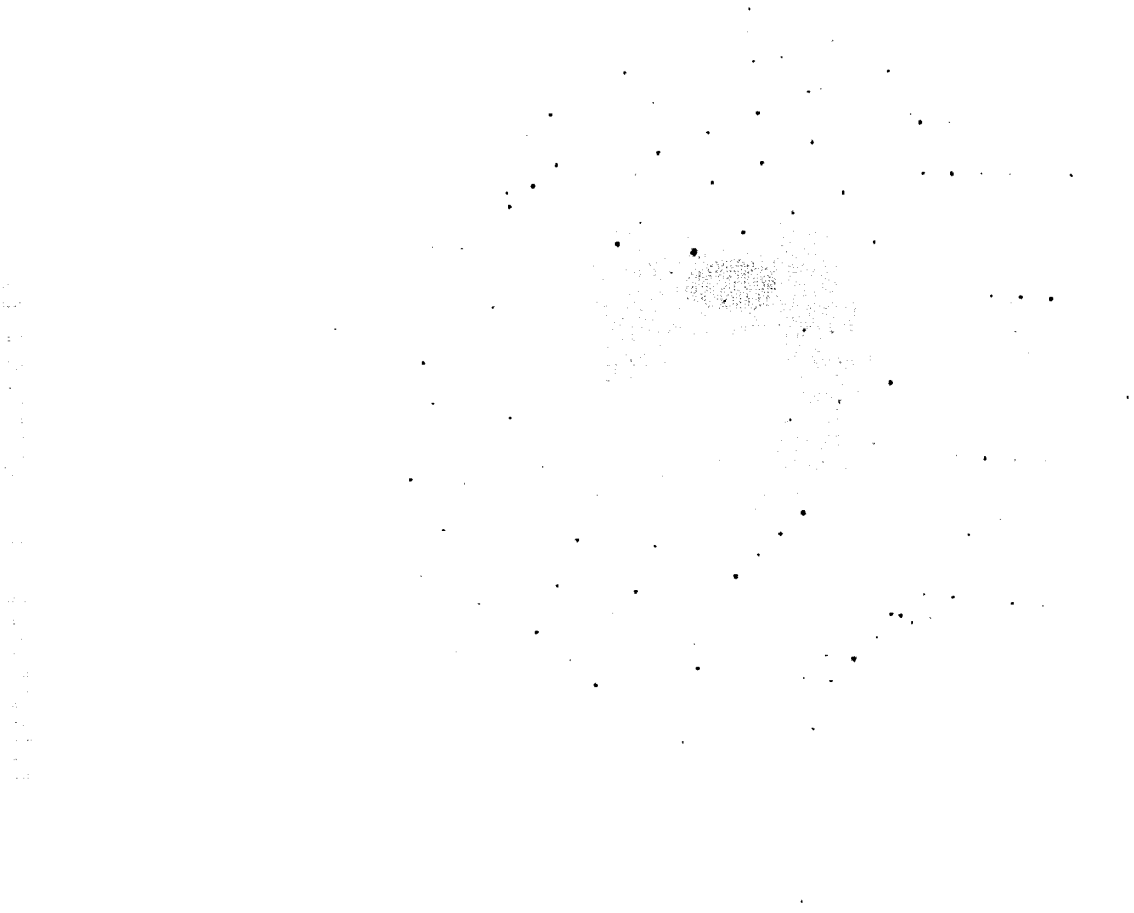


FIG. 6A Ribbon diagrams of the D. radiodurans LuxS protein, molecule A.

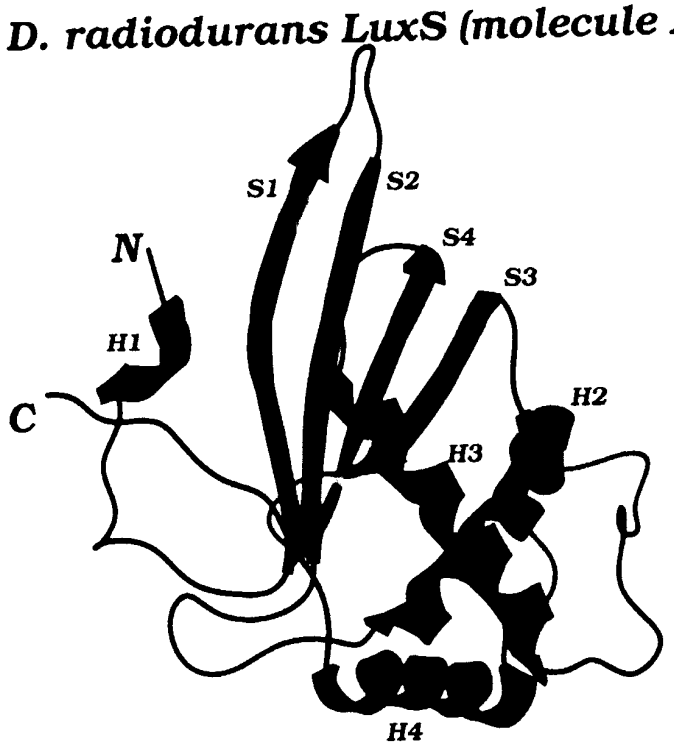
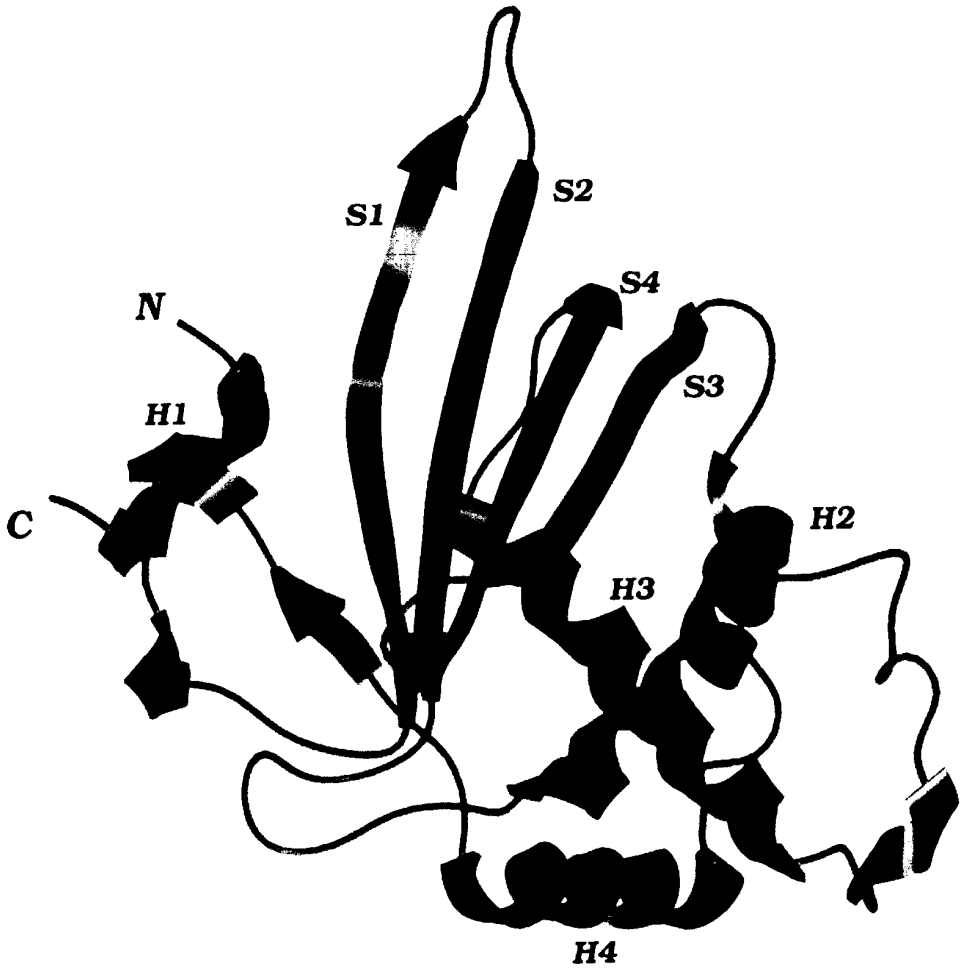
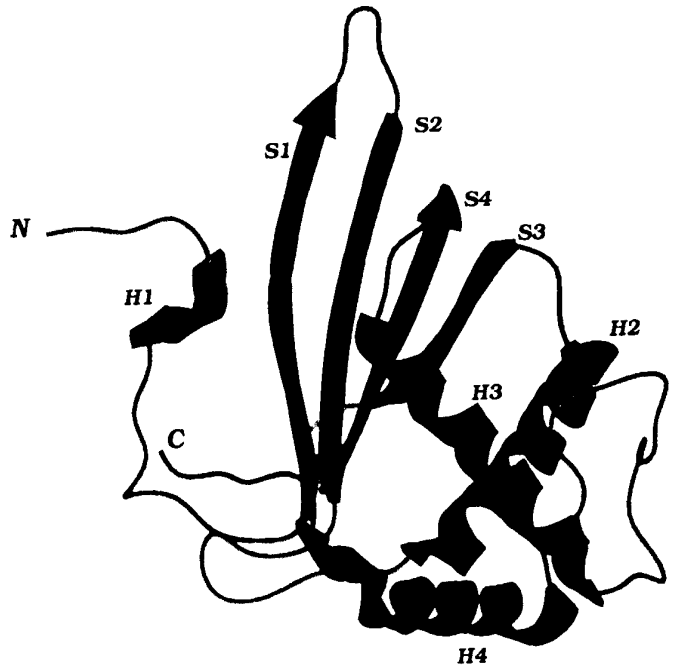


FIG. 6B Ribbon diagrams of the H. influenzae LuxS protein, molecule A.



H. influenzae LuxS (molecule A)

FIG. 6C Ribbon diagrams of the H. pylori LuxS protein, moleculeB.



H. pylori LuxS (molecule B)

FIG. 7A Ribbon diagram of H. pylori LuxS as a dimer, the contents of the asymmetric unit.

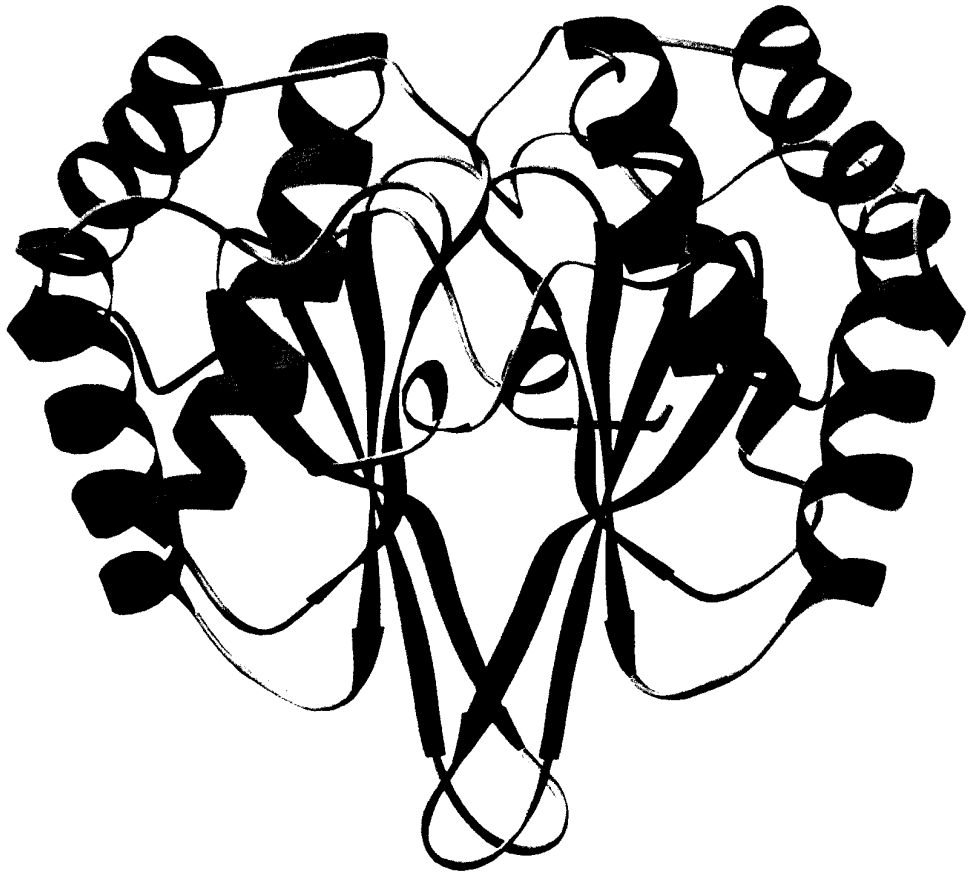


FIG. 7B Ribbon diagram of H. influenzae LuxS as a dimer with the bound methionines indicated in ball and stick.

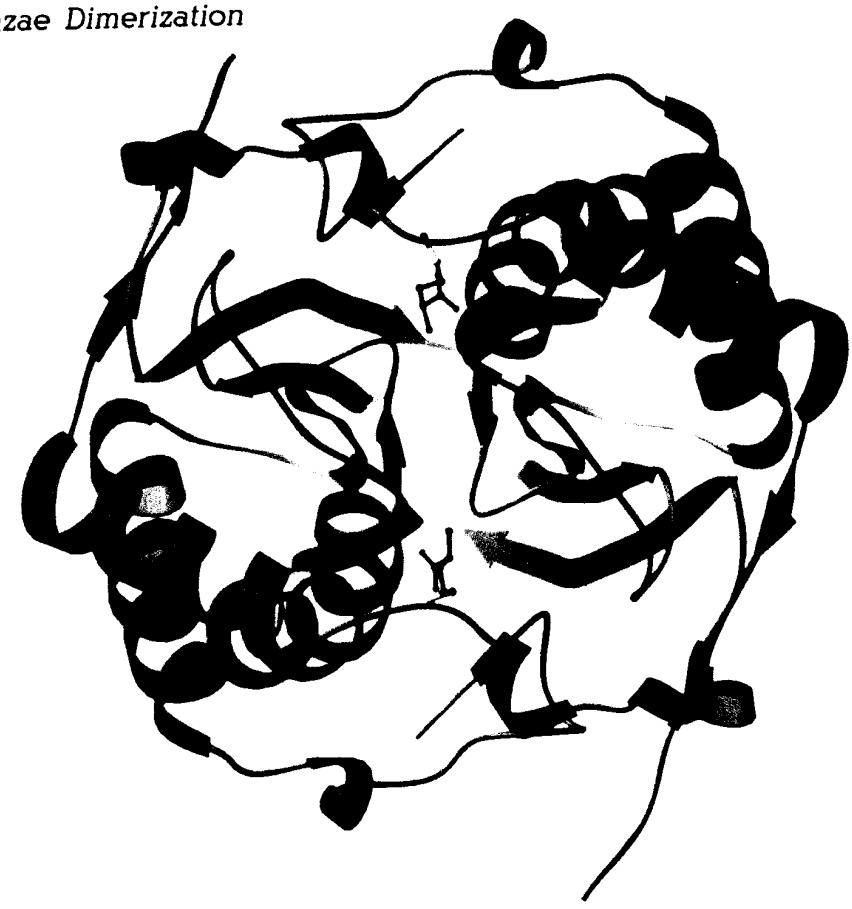


FIG. 8. Stereo image of C-alpha backbone of the H. pylori LuxS protein (same orientation as in FIG. 2A)

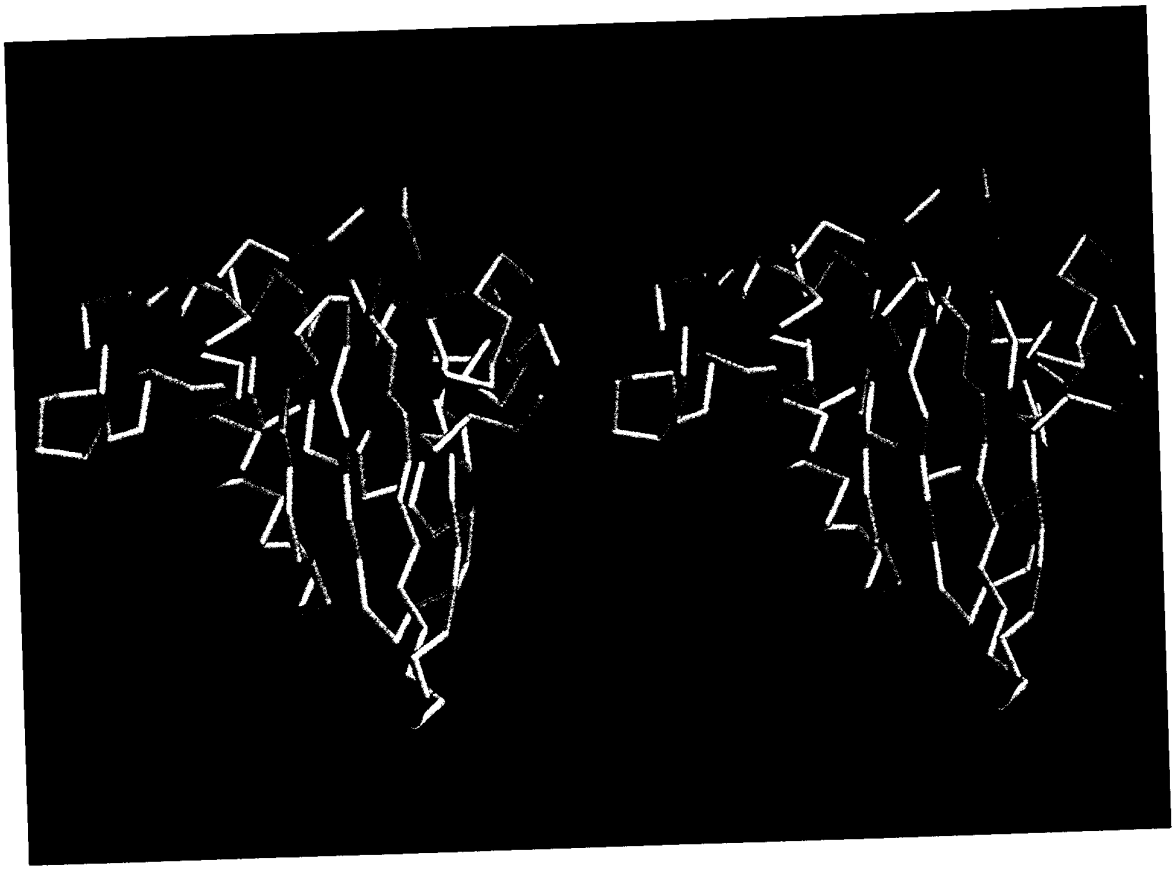


FIG. 9A Region of high sequence variability in LuxS as represented by Helix 3 (see FIG. 1). Helix 3 is the central (diagonal) helix closest to the observer.

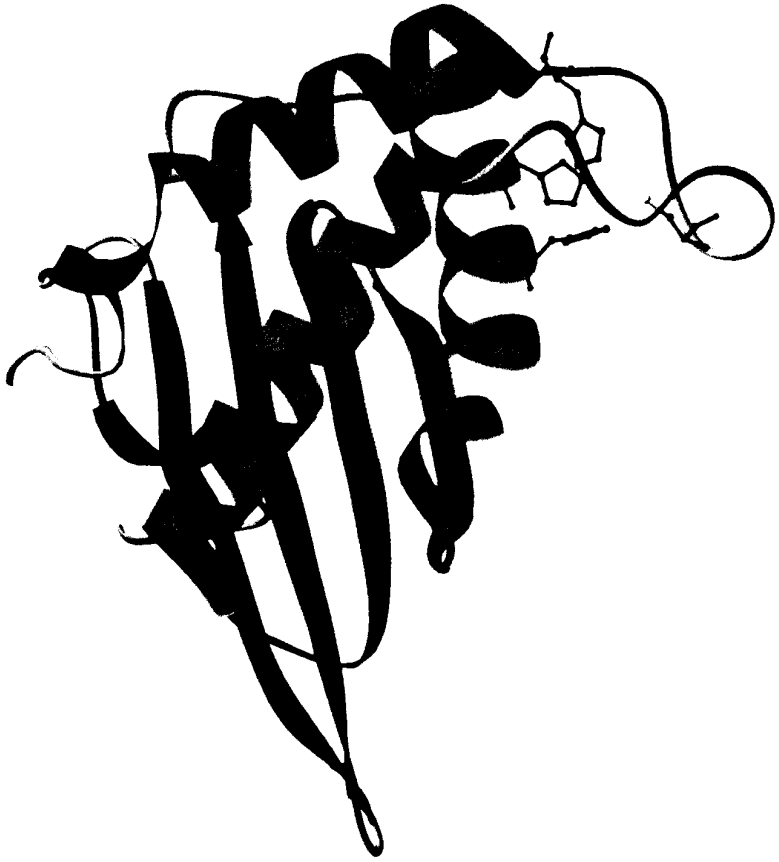


FIG. 9B Region of high sequence conservation in LuxS as represented by Helix 2 (see FIG. 1). Helix 2 is the central (vertical) helix closest to the observer.

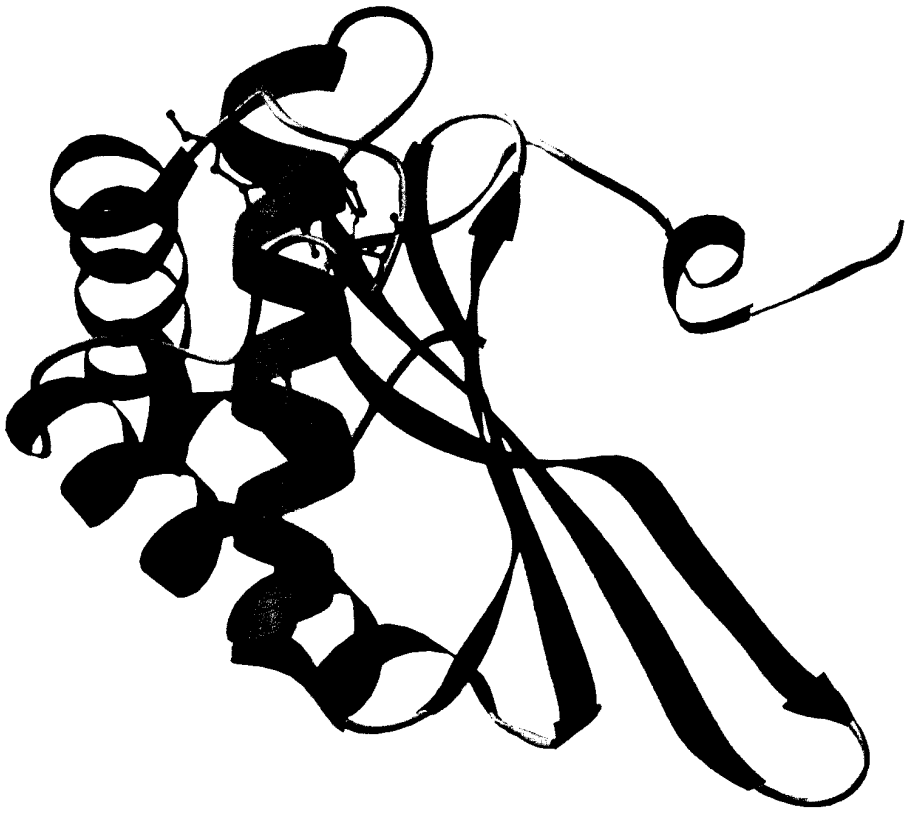


FIG. 10A The putative active site of LuxS.

FIG. 10B The active site may enlarge through dimerization of LuxS molecules in vivo, as illustrated by the dimer found in the asymmetric unit of the LuxS crystal.

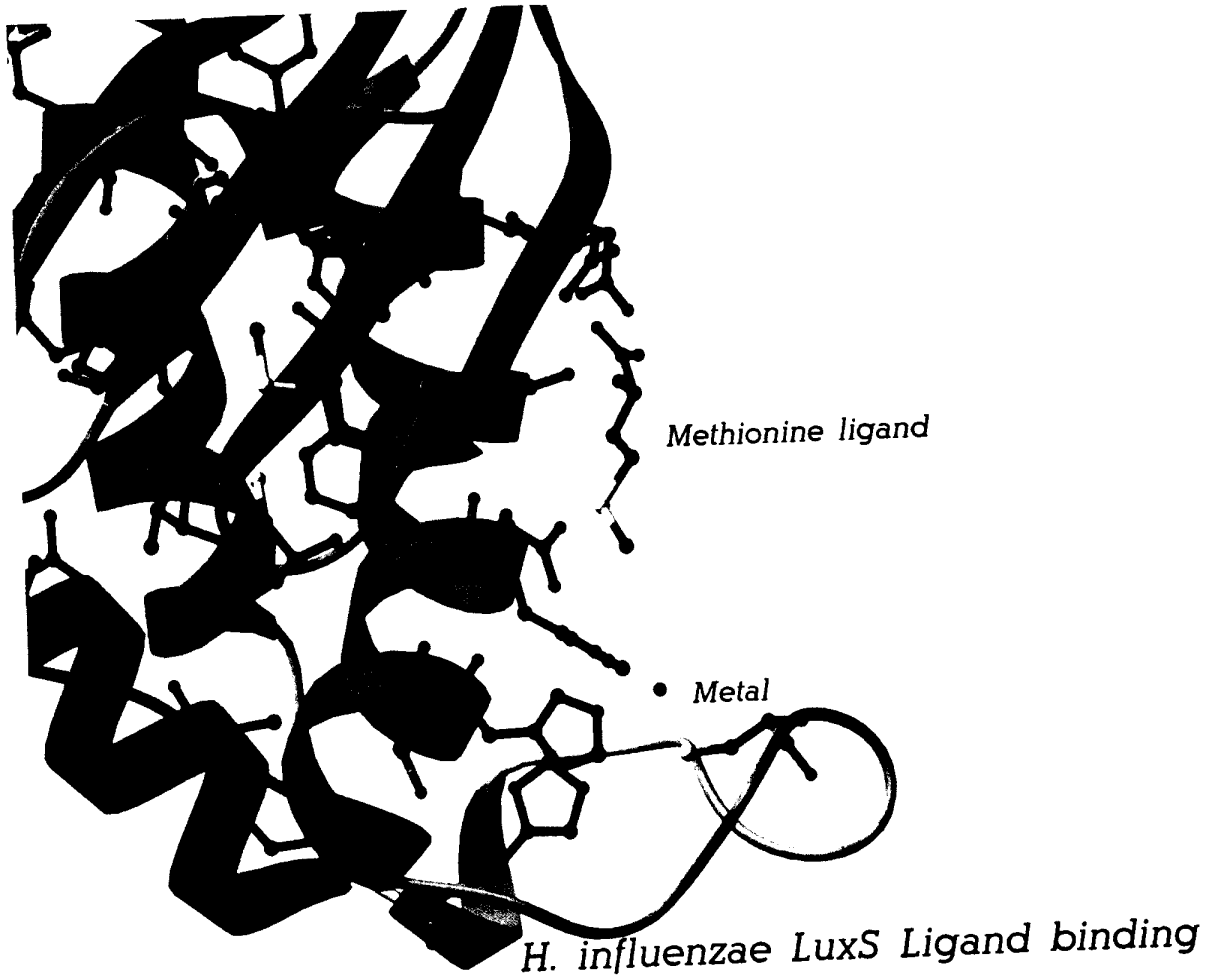


FIG. 11. Proximity of methionine binding site to metal binding site.

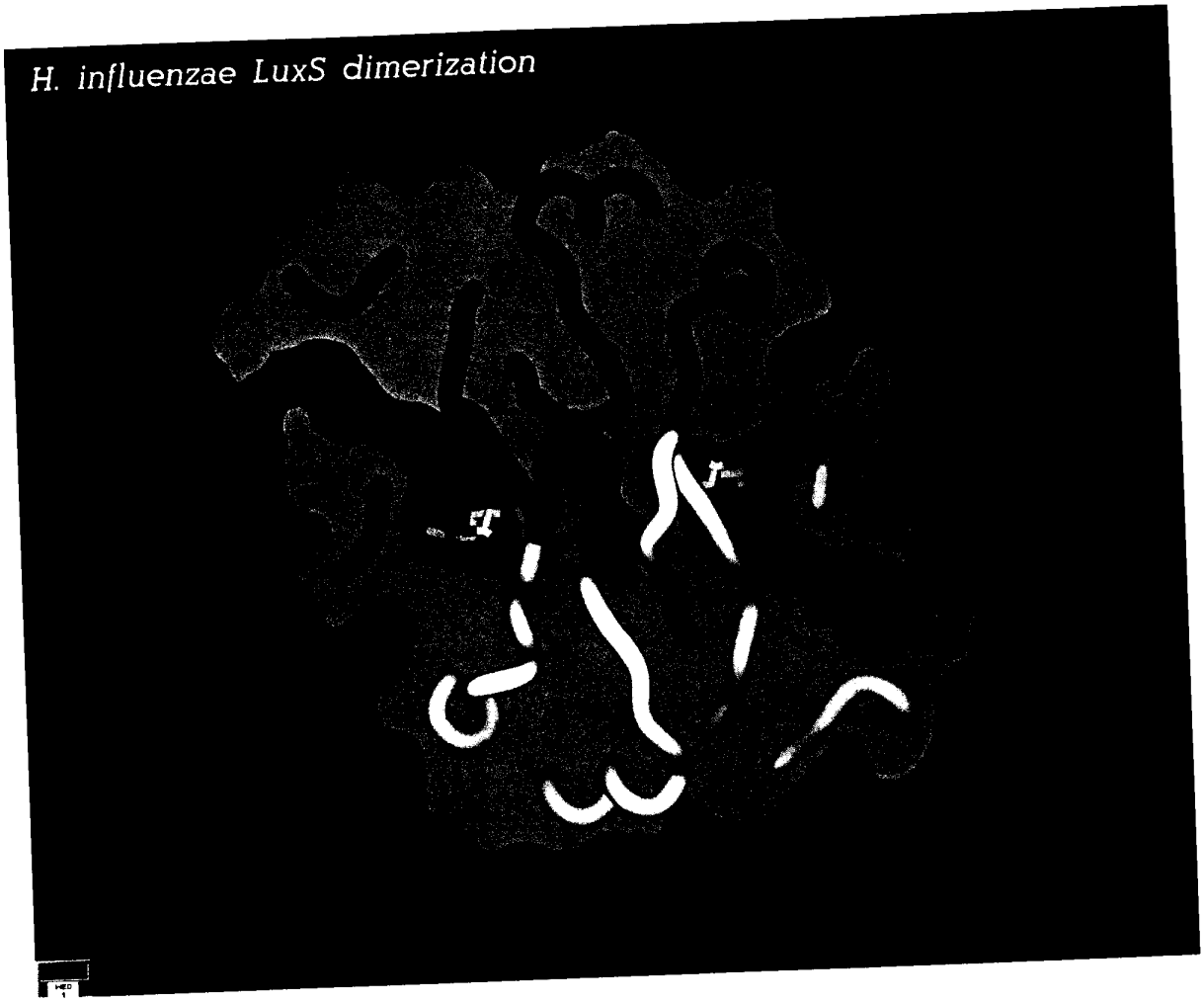


FIG. 12. SPOCK diagram of the molecular surfaces of the two molecule in the asymmetric unit of H. influenzae LuxS, cut away partially to reveal binding of the methionine ligands (ball and stick) and a channel through the opposing monomer leading out to the surface. A second channel to the binding site can also be seen. Worms represent the backbone atoms of the proteins in the cut away region.

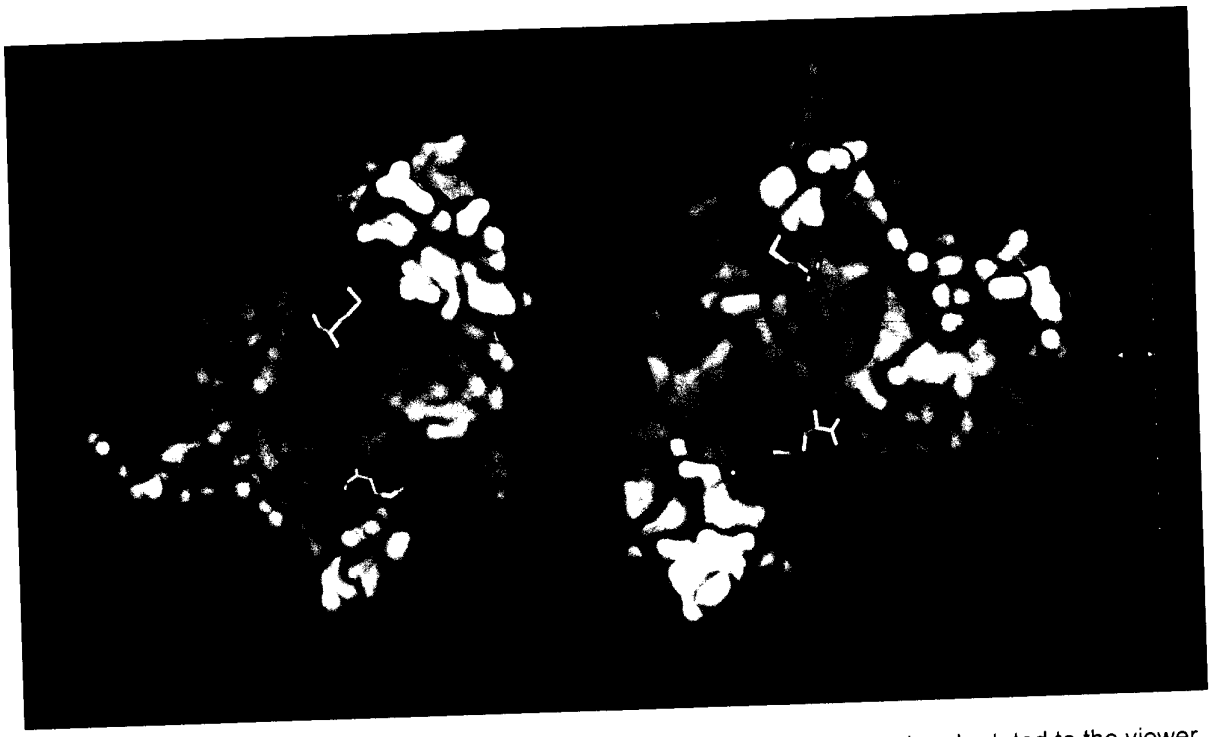


FIG.13A Molecular surface diagram of the H. influenzae LuxS dimer, separated and rotated to the viewer. The methionine ligand are represented as ball and stick, one per monomer with the virtual gold ligands representing where the methionine would lay across the opposing molecule. Red represent negative potential and blue positive potential. The charge complementarity of the dimerization is clear.

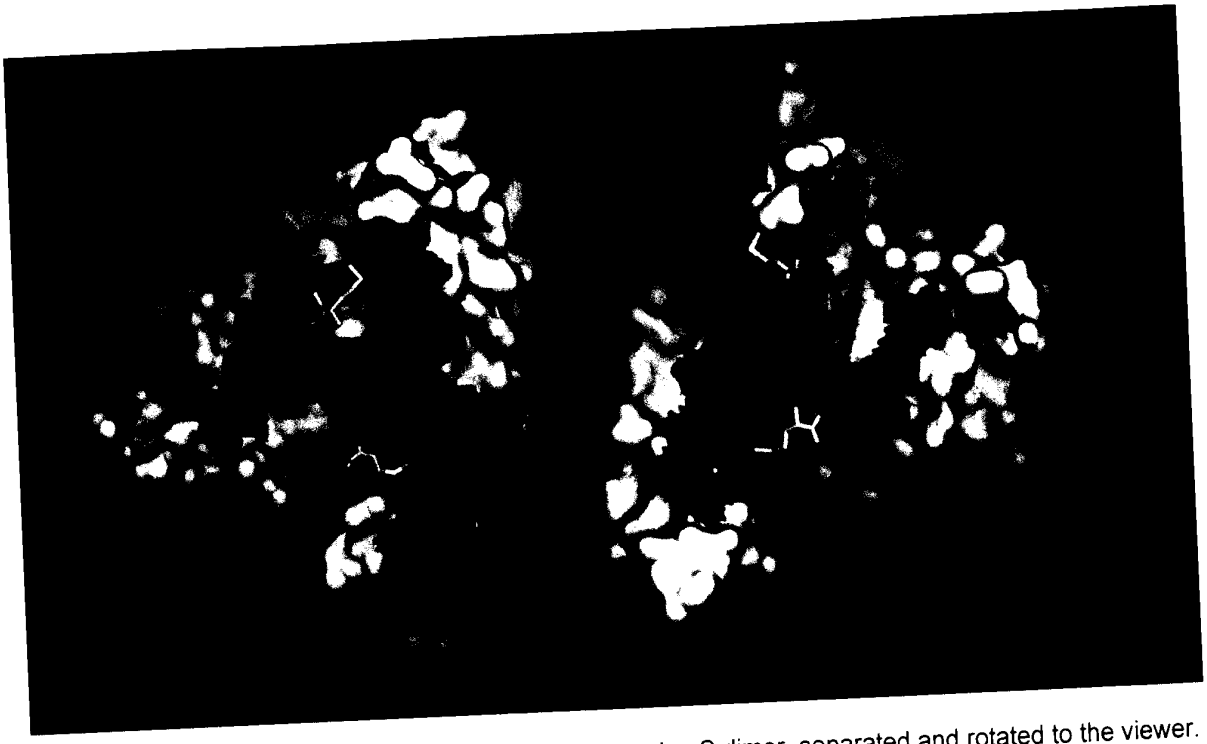


FIG. 13B Molecular surface diagram of the H. influenzae LuxS dimer, separated and rotated to the viewer. The methionine ligand are represented as ball and stick, one per monomer with the virtual gold ligands representing where the methionine would lay across the opposing molecule. Green represents conserved hydrophobic residues and red other conserved residues in the LuxS family (same as the color coding in FIG. 1).